MITlaos User Manual

Version 2.1 Beta for MATLAB

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Introduction

This manual describes the use of **MITlaos** (MATLAB version) for analyzing rheological properties in large amplitude oscillatory shear (LAOS). In addition to calculating standard viscoelastic parameters such as G_1', G_1'', **MITlaos** calculates additional parameters for interpreting nonlinear viscoelastic behavior. Brief definitions and interpretation of these nonlinear viscoelastic parameters are given in Appendix A. For detailed information regarding definitions and interpretation please refer to Cho *et al.* (2005), Ewoldt *et al.* (2006), and Ewoldt *et al.* (2007a).

Installation of MITlaos

MITlaos is currently distributed as a ZIP folder which contains multiple subfolders and multiple MATLAB subfunctions. Installation is done by unzipping and saving the **MITlaos** folder to any location on the local hard drive. Although any location is acceptable, a convenient location for the **MITlaos** folder is ...\MATLAB\work\MITlaos.

WARNING: Do not modify the contents of the **MITlaos** folder. Please contact MITlaos@mit.edu regarding installation problems.

Running MITlaos with MATLAB

Structure of Input Data File

MITlaos requires a text-based (ASCII) data file which contains columns of data. Header information is typically tolerated by the program. At a minimum, time-series data for strain (or displacement) and stress (or torque) are required. Additionally, a data column of time may be included if data are sampled at uneven intervals.

NOTE: **MITlaos** is flexible regarding the arrangement of columns in the data input file. The user will specify which column contains strain, stress, and time (optional).

Running the Program

Once **MITlaos** is installed and the data input file is of the proper form, **MITlaos** can be initialized with the following sequence.

1. Open MATLAB
2. Change the current working directory to the **MITlaos** folder (e.g. ...\MATLAB\work\MITlaos\). This folder should contain MITlaos.m
3. Type MITlaos at the command prompt to start the program

Main Window Overview

The **MITlaos** program consists of one main window (Figure 1) and several side windows. The main window shows all the necessary steps for analyzing sets of data. Several buttons in the main window open side windows that provides the user with more information and with more options to customize the data analysis.

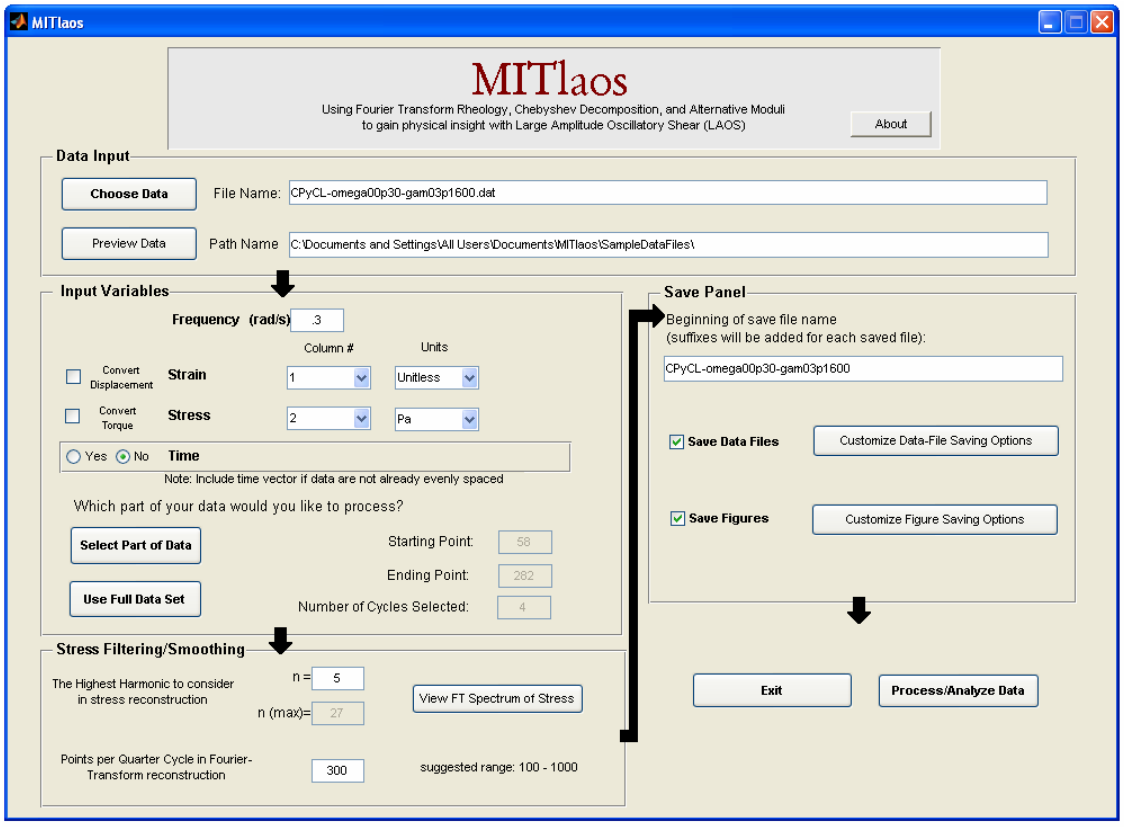

Figure 1: The **MITlaos** main window (arrows added to show the standard order of completion)

The **MITlaos** main window is broken into separate panels (which look like boxes) that group together related information. **MITlaos** was designed for filling out the information in one panel and then moving to the next one. The typical order for using **MITlaos** is to complete the Data Input panel and then the Input Variables panel, the Stress Filtering/Smoothing panel (optional), the Save Panel (optional), and then to press the 'Process/Analyze Data' button. The black arrows in Figure 1 show the progression across the main **MITlaos** window. This User Manual will also follow this order.

Data Input Panel

The Data Input panel lets the user select and preview the data file **MITlaos** will analyze. To select the data file, either click the Choose Data button or type the filename and its directory into the File Name and Path Name boxes (see Figure 2).

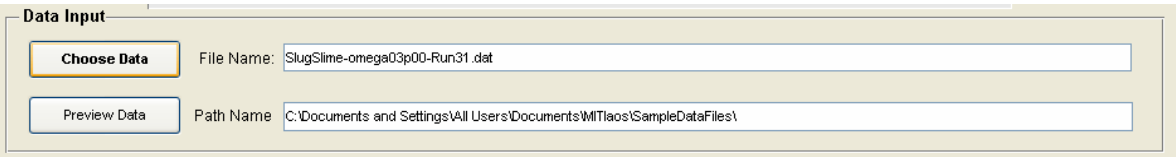

Figure 2: Data Input Panel

Choose Data button

Press the 'Choose Data' button in the Data Input panel to browse and select the file to analyze (Figure 3). Select the file, then click 'Open' and the filename and directory information will automatically be entered into the **MITlaos main window**.

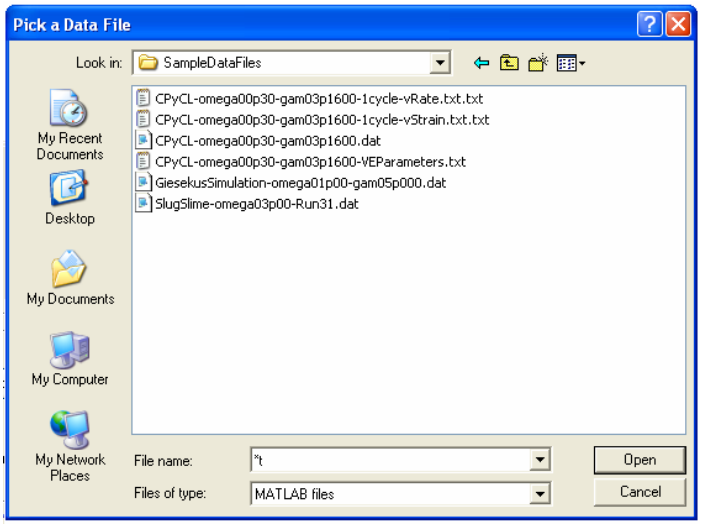

Figure 3: Choose Data Window

Preview Data button (Optional)

The 'Preview Data' button uses a function called Import Wizard to preview the selected data file. This can be used to quickly look at the contents of the selected input file. The Import Wizard is shown in Figure 4.

> WARNING: Import Wizard must only be used for previewing data. Press 'Cancel' when finished using the wizard; DO NOT click 'Next.'

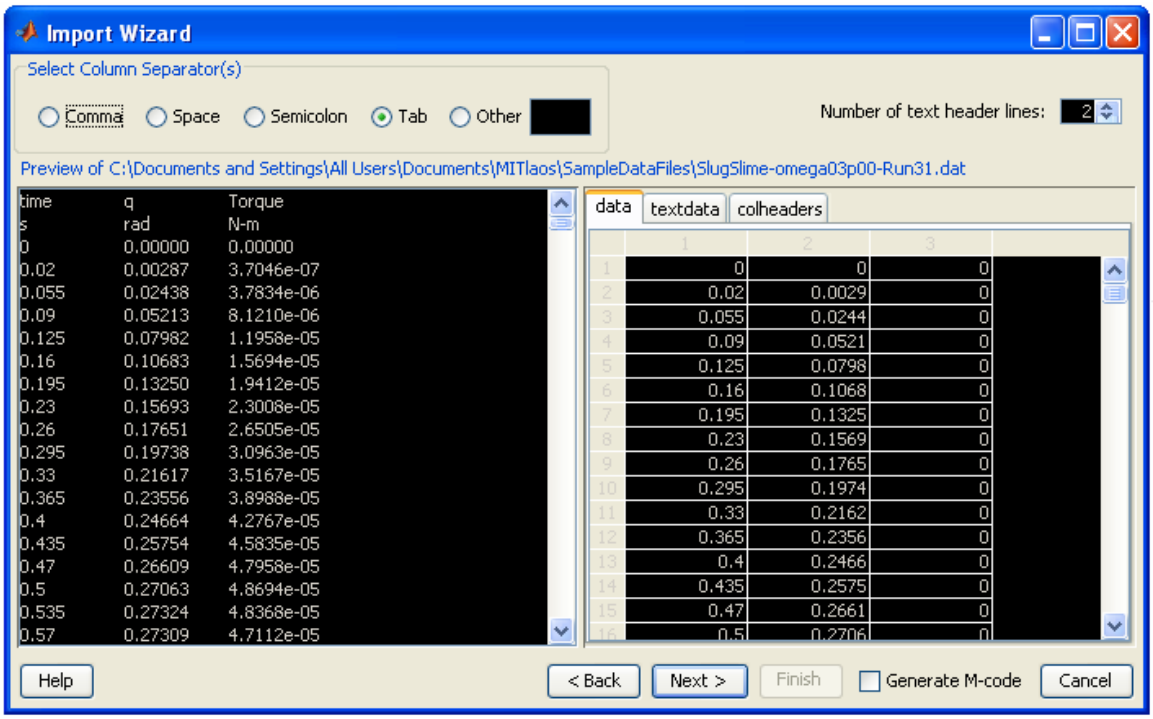

Figure 4: Import Wizard (only used to preview data)

In Figure 4, the box on the left shows the raw contents of the chosen data file. The grid on the right shows how **MITlaos** will load the file. In the example shown in Figure 4, **MITlaos** automatically cuts off the top rows of text containing the headers and units and reads only the numerical data below them. Note that the values of Torque are being read properly, however the numerical value is so small that Import Wizard rounds to 0 in the display.

> ⚠ WARNING: Any options changed using The Import Wizard will NOT be changed in **MITlaos**. Import wizard is for previewing purposes only. If **MITlaos** does not properly read the input file, then the input file layout must be modified outside of **MITlaos.**

File Name edit box

The File Name edit box displays the name of the chosen data input file. Using the 'Choose Data' button will automatically fill in this box; however, the user may also manually type the name of the data file into this box if desired.

Path Name edit box

The Path Name edit box displays the directory of chosen input file. As with the File Name edit box, the 'Choose Data' button can be used to automatically fill in this box. The user also has the option to type the pathname of the data file into this box.

Input Variables Panel

The Input Variables panel allows the user to specify all the information **MITlaos** requires for loading the data. It asks three separate questions:

- At what oscillatory frequency was the sample tested?
- Which columns in the data file contain which variables?
- What portion of the time-series data should be analyzed?

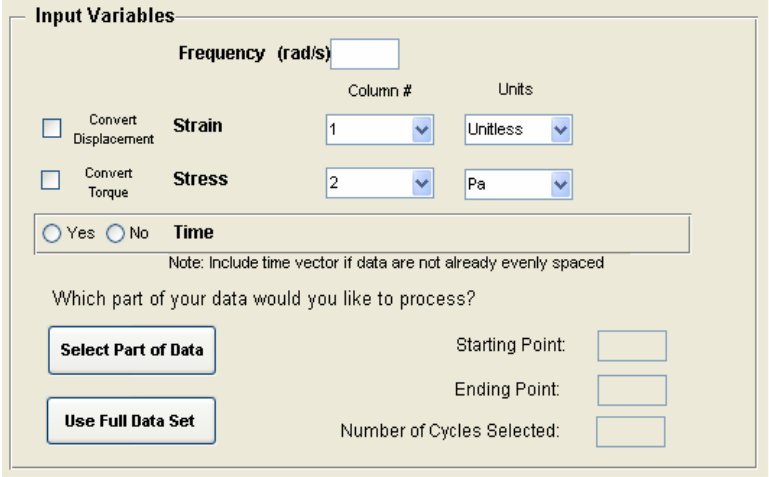

Figure 5: Input Variables panel

Frequency edit box

In the Frequency box, enter the oscillatory strain frequency used to test the sample, in units of [rad/s]. This input is necessary to run the analysis. It is suggested that the user include the frequency in the input filename as a convenient reference.

Column Specification

Since different kinds of rheometers have different formats for saving data, **MITlaos** is flexible in how it can read raw data. To change which column in the data file is read as strain, click on the dropdown menu to the right of the word 'Strain' and underneath the heading 'Column #'. If '2' is chosen from the dropdown menu, the second column in the input data file will be read as strain. Similarly, one can select which column is read as 'Stress' and which column is read as 'Time.' To make the Time column options visible, the user must first select the 'Yes' box to the left of the word 'Time'. If the input datafile has headers labeling the columns, it is possible to see them with the 'Preview Data' button (in the Data Input panel) to see which column contains which variable.

NOTE: Different columns must be selected for each variable.

Strain and Stress are the two variables required by **MITlaos**. Time is an additional variable that can be incorporated into the analysis if necessary. If the data was NOT collected at equally spaced time intervals, then it is important to include time as an input. If time is not included, **MITlaos** will assume the data points are equally spaced in time. It is recommended to NOT include time if data are evenly spaced.

In order to input displacement (instead of strain), click on the 'Convert Displacement' checkbox to the left of the word 'Strain'. A box allowing the input of a conversion factor will appear to the right of 'Units', and the word 'Strain' will be changed to 'Displacement' (Figure 6). Use the appropriate conversion factor such that strain is *unitless* (i.e. *not* in terms of percent), according to the equation $\gamma[-] = F_\gamma \Theta$.

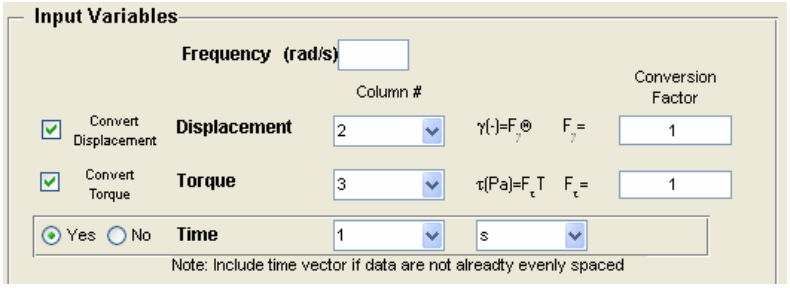

Figure 6: Input Variables panel, with 'Convert Displacement' and 'Convert Torque' options selected, and the 'Time' column input turned on

If the data was collected as torque, instead of stress, click on the 'Convert Torque' box to the left of the word 'Stress'. Similar changes will occur, allowing the user to specify a conversion factor between torque and stress. Use the appropriate conversion factor such that stress is in units of Pascals, according to the equation $\tau[\mathrm{Pa}] = F_\tau T$. Note that torque may be reported in various units, but F_τ *must* be chosen to give stress in units of Pascals. These conversion factors depend on the type and size of geometry being used (cone-plate, plate-plate, etc.). Values for conversion factors may be found in rheology textbooks, and may sometime be given by the geometry manufacturer.

Data Windowing

MITlaos can analyze all or part of the time-series data contained in the input file. There are two large buttons, titled 'Select Part of Data' and 'Use Full Data Set' that allow the user to choose between these options (see Figure 5). To the right of these buttons are three boxes which display the starting point, ending point, and number of cycles chosen from the dataset. These boxes will be empty if no data range has yet been chosen.

NOTE: At least one complete cycle must be selected for the analysis to work properly

To analyze the full time-series data set, press the 'Use Full Data Set' button. The full dataset will be trimmed to an integer number of complete cycles (this is necessary for analysis), and the boxes to the right of the button will immediately display how much data will be included for analysis.

Windowing the data is required if the time-series data contain transients, or if several strain amplitudes or frequencies are contained within the same data. In these cases, only part of the data should be used for each analysis. Press the 'Select Part of Data' button and a new window will open called 'processPartDataGUI', which allows the user to select which portion of the time-series to include for analysis.

ProcessPartDataGUI

Stress and strain are plotted against time (or arbitrary time) in the ProcessPartDataGUI (Figure 7). Since **MITlaos** is designed to analyze a viscoelastic system response to a sinusoidal strain input, the strain signal should appear as a sine wave and the stress response should oscillate with the same period (note that stress should simply be a shifted sine wave in the linear viscoelastic regime). By looking at this stress and strain signals, the user should be able to determine which portion of the data should be analyzed.

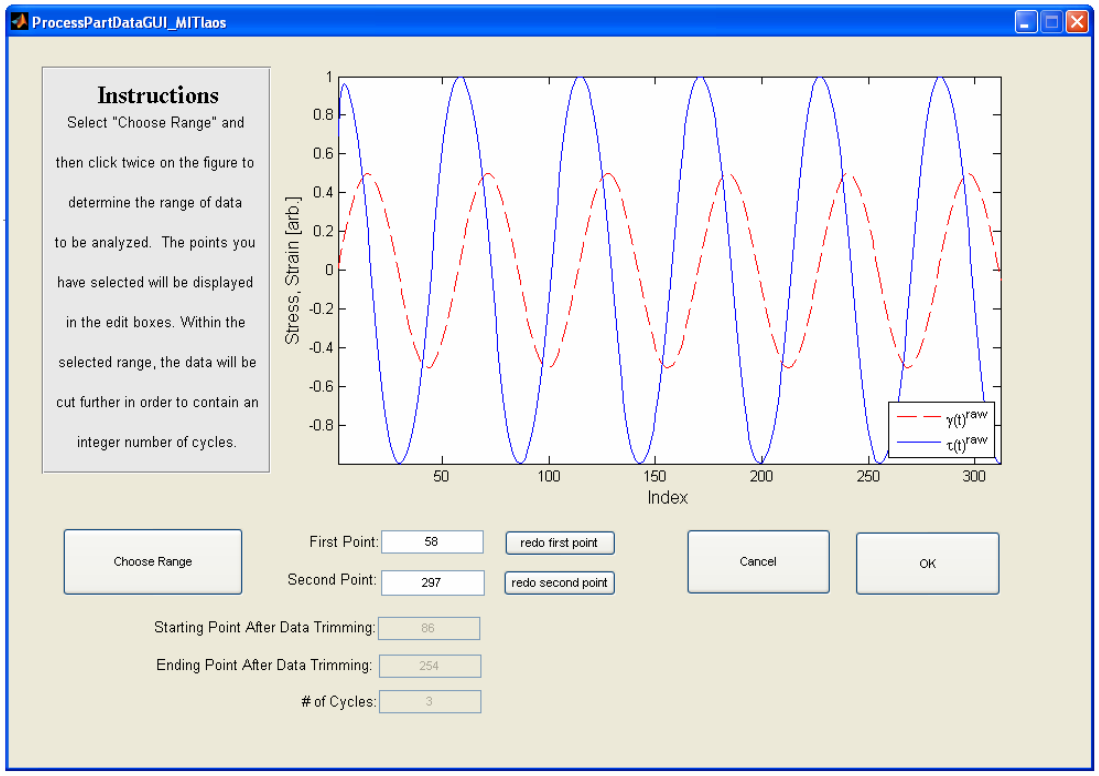
ProcessPartDataGUI_MITlaos
Instructions
Select "Choose Range" and then click twice on the figure to determine the range of data to be analyzed. The points you have selected will be displayed in the edit boxes. Within the selected range, the data will be cut further in order to contain an integer number of cycles.
Stress, Strain [arb.]
Index
γ(t)raw
τ(t)raw
Choose Range
First Point: 58
redo first point
Second Point: 297
redo second point
Cancel
OK
Starting Point After Data Trimming: 86
Ending Point After Data Trimming: 254
# of Cycles: 3

Figure 7: ProcessPartDataGUI window

Click the 'Choose Range' button on the bottom left of the window to select the desired portion of data to analyze. The cursor will immediately change to a cross hair which will be used for selecting the limiting points of the desired range. Move the cross hair over the graph and click once at the beginning and once at the end of the desired data range (note that the vertical position of the crosshairs is irrelevant). The two chosen points will be displayed in the First Point, and Second Point edit boxes. If desired, the user may choose to manually type the location of the chosen points into the edit boxes.

The chosen data range will be further trimmed to be an integer number of cycles. The new limits of the data to be processed will be displayed in the 'Starting Point After Data Trimming' and 'Ending Point After Data Trimming' boxes. The bottom box shows the total number of complete cycles that will be used in data analysis. An integer number of cycles is required for proper processing.

It is possible to redo either of the endpoints of the initially selected data range. To redo one point, but leave the other point as is, click 'Redo First Point' or 'Redo Second Point' and then click on the graph. When satisfied with the selected data range, click 'OK'.

On Selecting The Data Range

The stress response reaches a steady state when the stress amplitudes of each cycle are equal and the shape of the cycle repeats itself. In Figure 7, steady state is reached after the first peak, which is slightly smaller than the others. For best analysis, include only cycles that have reached equilibrium.

Example: Incorrect column settings

To illustrate a possible mistake with the settings of the Input Variables panel, a sample picture is included here (Figure 8) in which the columns for the data have been incorrectly assigned. As shown in Figure 8, a straight line running through the graph is an immediate indication that something is wrong, since both stress and strain should be oscillating. In this example the time column was incorrectly specified as the strain column.

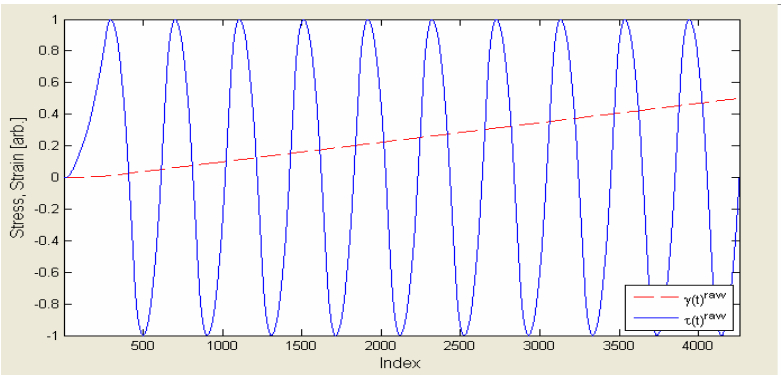

Figure 8: Data Set with Incorrectly Specified Columns

Example: Multiple strain-amplitudes in one data file

Figure 9 shows an example of more advanced data processing that can be done with **MITlaos**. This shows the data collected from a waveform test combined with a stepwise increases in amplitude (6 cycles at each strain-amplitude). The decreasing stress amplitudes after each step show that the system has not reached equilibrium. **MITlaos** can not accurately process this entire set of data (Figure 9) due to the changing strain-amplitude. However, the data can manually be windowed to analyze one strain-amplitude at a time. This data set could then be used to separately analyze four different strain amplitudes. Note, however, that for best results it is recommended that the analysis can be carried out on a system that has reached steady state.

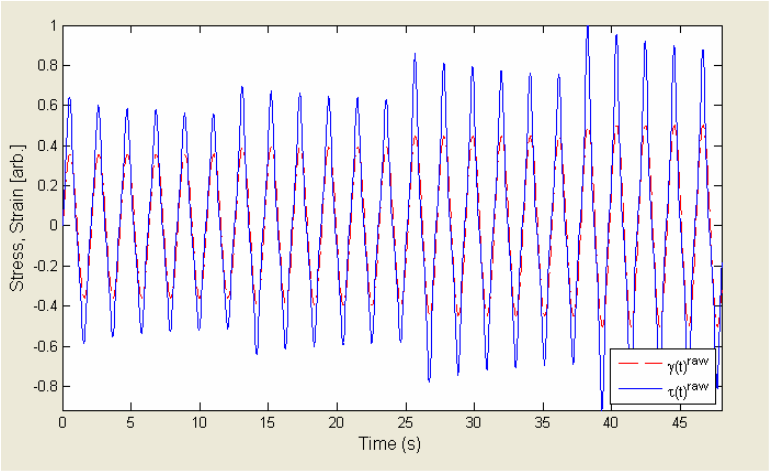

Figure 9: Data Set with a Stepwise Increase in Amplitude

Example data files are included with the distribution of **MITlaos** in the subfolder …\MITlaos\subfunctions_MITlaos\. A document in the same subfolder describes these example data files.

NOTE: The following 2 sections (Stress Filtering/Smoothing panel and Save panel) are OPTIONAL steps. Default values for these settings are provided when **MITlaos** is initialized. However, these settings are not optimal for all data.

Stress Filtering/Smoothing Panel

Stress signals are smoothed with the help of a Fourier Transform (FT). The raw stress signal is first decomposed into Fourier components. A linear viscoelastic response should have only one frequency component in its Fourier spectrum, whereas a nonlinear viscoelastic response will also contain higher harmonics. The smoothed stress signal is then reconstructed using only the odd, integer harmonics of the Fourier spectrum, since all other harmonics are the consequence of noise, unsteady oscillations, or systematic bias. This FT filtering technique eliminates noise and also aids in calculating nonlinear viscoelastic parameters. The Stress Filtering/Smoothing panel allows the user to change two options involved in this Fourier reconstruction (Figure 10).

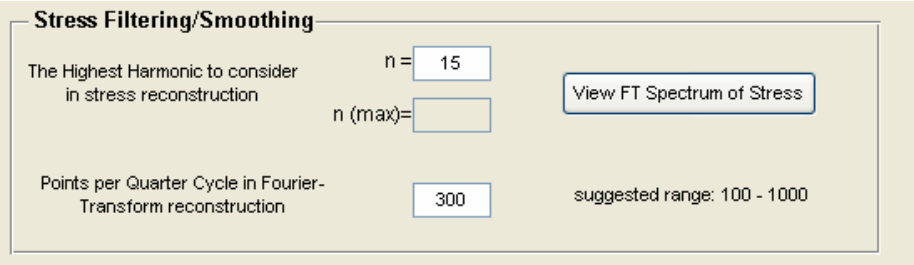

Figure 10: Stress Filtering/Smoothing panel

The first editable setting is the value for n, the highest odd harmonic used in stress reconstruction (i.e. $\omega_{max} = n\omega$, where ω is the oscillatory test frequency). The maximum available value for n, labeled as 'n (max)' is displayed as well (this indicates the Nyquist frequency). The value of 'n (max)' is limited by the number of data points per cycle, and will be displayed as soon as a data range is chosen (see data windowing). Although 'n (max)' is the maximum possible value for n, it is common to use a lower n value than this.

Choosing a lower n will limit the number of harmonics used in the Fourier Transform (FT) reconstruction. If n is too low, the stress will be overly-smoothed and less accurate. However, if n is too high, random noise may be incorporated into the smoothed stress. For help on choosing the appropriate value for n, click the 'View FT Spectrum of Stress' button (see below).

The second editable setting is the 'Points per Quarter Cycle (PPQC) in Fourier-Transform reconstruction'. This value indicates the number of data points included in the reconstructed stress signal. A smaller number of points will decrease the resolution of the reconstruction, and a higher number of points will increase the file size. The default value is currently 300 PPQC, which is likely adequate to capture most nonlinearities. No limit is placed on size of the reconstructed Fourier-Transform, other than the operator's ability to store the resulting data. Note that a smoothed stress signal with a large PPQC value will likely represent a higher time-resolution than is actually contained in the smoothed signal, since harmonics greater than n have been omitted.

View FT Spectrum of Stress button

Clicking the 'View FT Spectrum of Stress' button opens the FTHamonicGUI window (Figure 11). This window displays the Fourier Transform (FT) power spectrum of the raw stress signal, and provides the user with information to choose the appropriate value for ***n***.

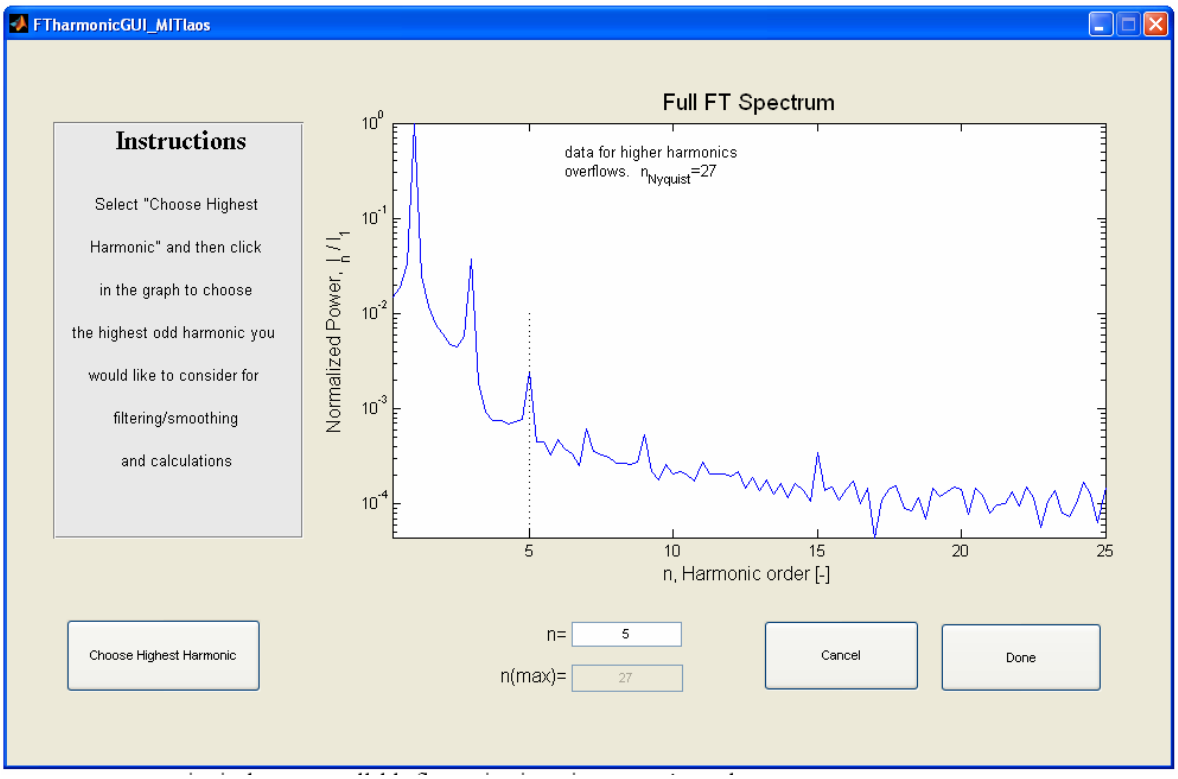

Figure 11: FTharmonicGUI window

The FT spectrum will typically show a series of decreasing peaks that eventually fall into the noise floor at higher frequencies (note that a single peak at n=1 is required for a linear viscoelastic response). Any data signal will have such a noise threshold. For Figure 11, the signal to noise ratio for the first harmonic is of the order S/N ~ 10^4.

An appropriate value for ***n***, the highest harmonic to use in reconstruction, is typically a value which is above the noise threshold, yet high enough to capture the viscoelastic nonlinearities. To select the desired ***n*** value, click the 'Choose Highest Harmonic' button. The pointer will turn into a set of crosshairs. Next, click on the graph at the desired ***n*** value, typically near the last big peak that stands out above the noise threshold (note that the vertical location of the crosshairs is irrelevant).

When the graph is clicked once, the value of n will automatically be rounded to the nearest odd integer and displayed in the box below the graph. The user may also manually type the desired value of ***n*** into this box.

Save Panel

The Save Panel allows the user to select all the options for saving the analyzed data as figures and/or data files. No files will be saved until the 'Process/Analyze Data' button is clicked, which is located at the bottom of the main window. The data will be saved at the completion of the analysis.

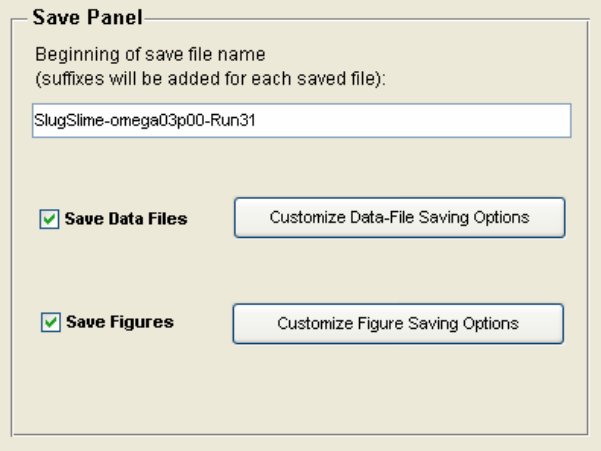

Figure 12: Save panel

The edit box at the top of this panel allows the user to choose the beginning of the save file names. When the figures and data files are saved, each of their names will begin with the text in this box, and an appropriate suffix will be added to distinguish each file. This provides a simple way to group related files together. For example, when saving a JPEG image called Figure1 (a setting located beneath the 'Customize Figure Saving Options' button), if the text the 'Beginning of save file name' box is 'TestSample42', then the final save file would be called 'TestSample42-Figure1.jpg'.

> NOTE: The saved files (figures and data files) will always be located in the same folder as the initial input data file.

The Save Data Files checkbox

This box must be checked to save any data files.

The Save Figures checkbox

This box must be checked to save any image files.

Details regarding the 'Customize Data-File Saving Options' and 'Customize Figure Saving Options' buttons are discussed in the following two subsections.

Customize Data-File Saving Options button

When the 'Customize Data-File Saving Options' button is clicked, the datasaveGUI window opens, allowing the user to specify the layout and format of the saved data files (Figure 13).

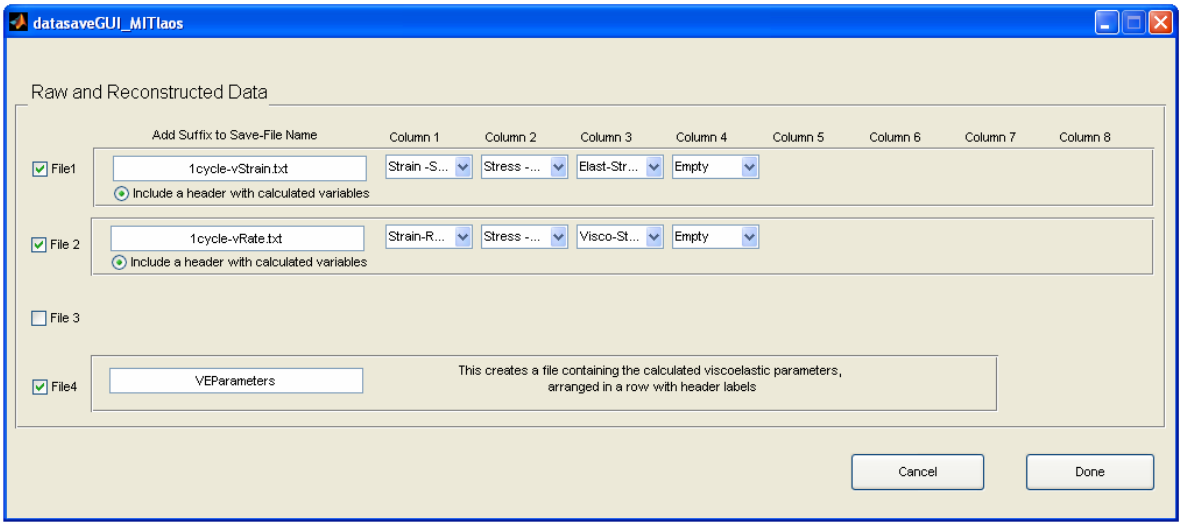

Figure 13: datasaveGUI window

The check boxes labeled 'File 1', 'File 2', etc. determine if each save will be saved. 'File 1', 'File 2', and 'File 3' are intended to contain columns of time-series data, the layout of which can be modified by using the dropdown menus associated with each file. 'File 4' has a fixed format, since it contains the calculated viscoelastic parameters. All data files will be saved with the extension .txt.

The layout 'File 1' will be determined by the box immediately to the right of the 'File 1' checkbox. The window shown in Figure 13 indicates here that 'File 1', 'File 2' and 'File 4' will all be saved. Since the 'File 3' checkbox is unchecked, it will not be saved and none of its information is displayed in the window.

The edit boxes underneath the header 'Add Suffix to Save-File Name' will determine the last part of the name this file is saved as. Note that the beginning of each save file name will be identical, and can be changed in the Main Window under the Save Panel. In Figure 13, 'File 1' will be saved under a name ending with '1cycle-vStrain.txt'.

Files 1-3 have selectable round circles labeled 'Include a header with calculated variables' located under the save file name edit boxes. When this option is selected, a 23 line header will be printed in the file which specifies all the calculated viscoelastic parameters of the processed data.

The 'Column #' drop down menus to the right allow the choice of time-series data to be saved in each column. The drop down menu underneath the words 'Column 1' and to the right of 'File 2' will change the first column saved in the second file. Up to eight different columns can be specified for each save file.

File 4 is permanently set to create a save file containing all the calculated viscoelastic parameters, and contains two rows of text. The first row includes a text description for each parameter and the second row contains the numerical values for each parameter. This layout was chosen so that other programs could be written to easily access these viscoelastic parameters.

NOTE: If the 'Save Data Files' checkbox in the main window is not checked, none of these files will be saved regardless of what options are chosen.

Customize Figure Saving Options button

The 'Customize Figure Saving Options' button opens the figuresaveGUI window (Figure 14). The check boxes on the left allow the choice of which figures to save. The dropdown menus underneath the header 'Image Format' allow the choice of saving each figure as JPEG or TIFF format.

The edit boxes underneath the header 'Suffix to Append to File Name' will determine the last part of the name for each file. Note that the beginning of each save file name will be identical, and can be changed in the Main Window under the Save panel. As prescribed in Figure 14, the overview plot will be saved under a name ending with 'Fig_Overview.JPEG'.

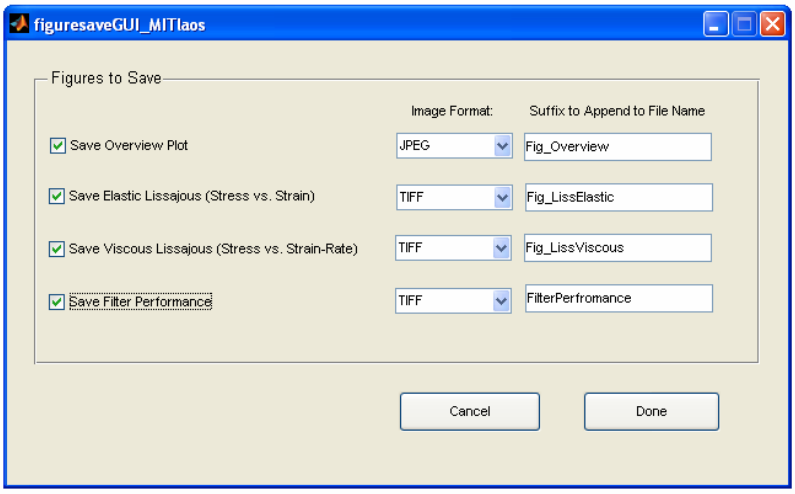

Figure 14: figuresaveGUI window

NOTE: If the 'Save Figures' checkbox in the main window is not checked, none of these figures will be saved regardless of the selected options.

Main Buttons

Once all of the details are specified, the analysis is initialized by clicking the 'Process/Analyze Data' button, at the lower-right corner of the **MITlaos** main window (Figure 15).

Figure 15: Main Program Buttons

Exit:
Quits **MITlaos** and closes main window.

Process/Analyzes Data:
This analyzes the selected data, using the chosen analysis options, and saves the specified figures and data files. Figures chosen for saving will also be displayed on screen for viewing.

Note that inputs in the **MITlaos** main window are only reset if **MITlaos** is closed and re-opened. This allows the user to

1. Tweak processing parameters, and quickly reprocess the data with the 'Process/Analyze Data' button

2. Select a different input data file while keeping the same processing parameters. This allows for quick subsequent processing of multiple data files.

Appendix A: Definitions of Nonlinear Viscoelastic Parameters

Alternative Viscoelastic Moduli

Since G_1', G_1'' are arbitrary and insufficient with nonlinear viscoelasticity, **MITlaos** uses two alternative ways to quantify elastic and viscous moduli of a complex material. All measures reduce to the linear moduli in the limit of small strain amplitude, but represent different approximations of the first order viscoelastic response. Different alternative moduli can be compared to quantify the type of nonlinearity (see below). Mathematical and graphical definitions of the elastic and viscous alternative moduli are given in Figure 16a and Figure 16b, respectively.

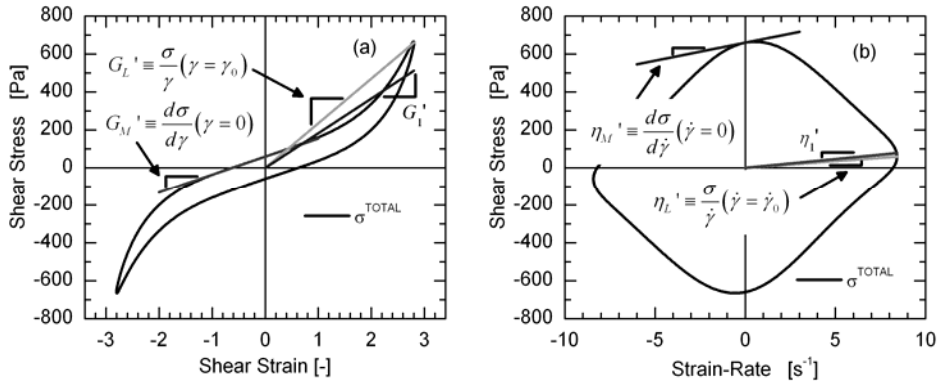

Figure 16. Definitions of alternative viscoelastic moduli, a) minimum-strain modulus G_M' and large-strain modulus G_L'; b) minimum-rate dynamic viscosity η_M' and large-rate dynamic viscosity η_L'. Figure reproduced from Ewoldt *et al.* (2007b).

The alternative viscoelastic moduli determined for a given equilibrium oscillatory response can be compared to indicate the nature of the viscoelastic nonlinearity, as summarized below.

$$\frac{G_L'}{G_M'}\begin{cases} >1 & \text{strain-stiffening} \\ =1 & \text{linear elastic} \\ <1 & \text{strain-softening} \end{cases} \qquad \frac{\eta_L'}{\eta_M'}\begin{cases} >1 & \text{shear-thickening} \\ =1 & \text{linear viscous} \\ <1 & \text{shear-thinning} \end{cases}$$

Viscoelastic Chebyshev Coefficients

For a strain-controlled oscillatory shear test, the nonlinear stress response is commonly decomposed as a Fourier series, shown below in two possible forms

$$\sigma(t;\omega,\gamma_0) = \gamma_0 \sum_{n\ \text{odd}} \left\{ G_n'(\omega,\gamma_0)\sin n\omega t + G_n''(\omega,\gamma_0)\cos n\omega t \right\}$$
$$\sigma(t;\omega,\gamma_0) = \dot{\gamma}_0 \sum_{n\ \text{odd}} \left\{ \eta_n''(\omega,\gamma_0)\sin n\omega t + \eta_n'(\omega,\gamma_0)\cos n\omega t \right\}$$

The total stress can be decomposed into "elastic" and "viscous" stresses by using symmetry arguments [Cho *et al.* (2005)].

$$\sigma'(x) \equiv \frac{\sigma(\gamma,\dot{\gamma}) - \sigma(-\gamma,\dot{\gamma})}{2} \quad \text{elastic} \qquad x = \gamma/\gamma_0$$
$$\sigma''(y) \equiv \frac{\sigma(\gamma,\dot{\gamma}) - \sigma(\gamma,-\dot{\gamma})}{2} \quad \text{viscous} \qquad y = \dot{\gamma}/\dot{\gamma}_0$$

Building upon the work of Cho *et al.* (2005), we suggest an additional orthogonal decomposition of the elastic and viscous stresses using Chebyshev polynomials of the first kind (see also Figure 17).

$$\sigma'(x) = \gamma_0 \sum_{n:\ \text{odd}} e_n(\omega,\gamma_0) T_n(x)$$
$$\sigma''(y) = \dot{\gamma}_0 \sum_{n:\ \text{odd}} v_n(\omega,\gamma_0) T_n(y)$$

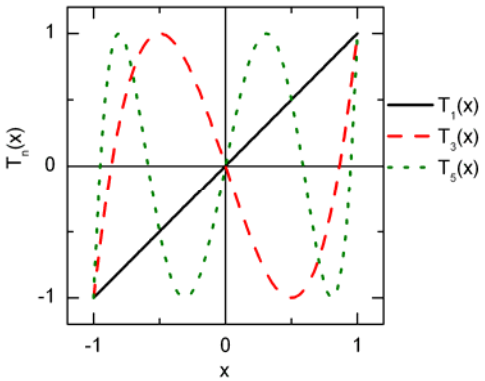

Figure 17: The first few odd Chebyshev polynomials of the first kind

The elastic and viscous Chebyshev coefficients are related to the oft-calculated Fourier Transform coefficients as

$$\begin{aligned} e_n &= G_n'(-1)^{\frac{n-1}{2}} \\ v_n &= \frac{G_n''}{\omega} = \eta_n' \end{aligned} \qquad n\text{:odd}$$

A positive third-order contribution results in higher stress at maximum strain (or strain-rate) than represented by the first-order contribution alone. Thus, the sign of the third-order coefficients suggest a physical interpretation of stiffening/softening and thickening/thinning, and are directly related to the Fourier coefficients. The interpretation of these parameters is summarized below.

$$e_3 = -G_3' \begin{cases} > 0 & \text{strain-stiffening} \\ = 0 & \text{linear elastic} \\ < 0 & \text{strain-softening} \end{cases} \qquad v_3 = \frac{G_3''}{\omega} \begin{cases} > 0 & \text{shear-thickening} \\ = 0 & \text{linear viscous} \\ < 0 & \text{shear-thinning} \end{cases}$$

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